Electronic Supporting Information

for

Guest Encapsulation and Coronene-C_{60} Exchange in Supramolecular Zinc Porphyrin Tweezers, Grids and Prisms

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NMR Spectra

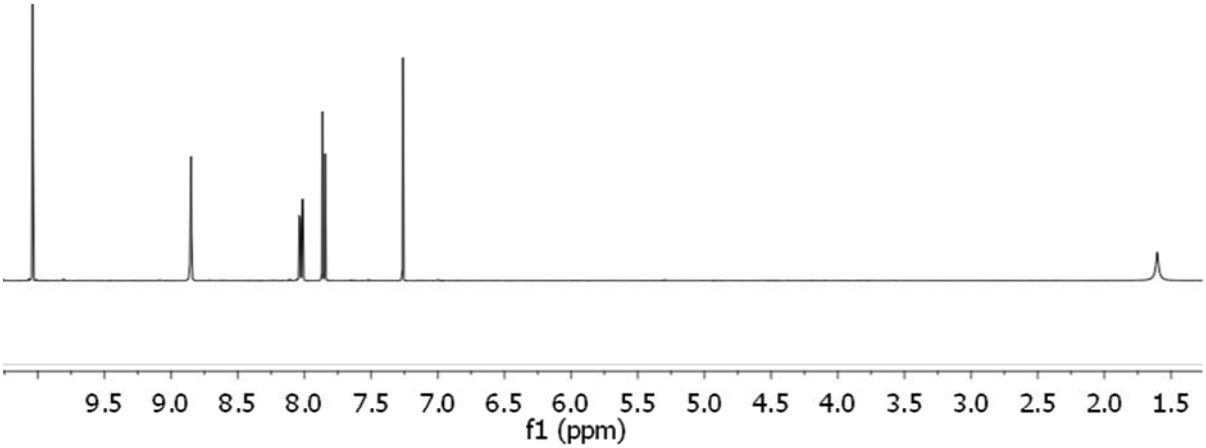

Figure S1. ^{1}H NMR of compound **4** ($CDCl_3$, 400 MHz, 298 K).

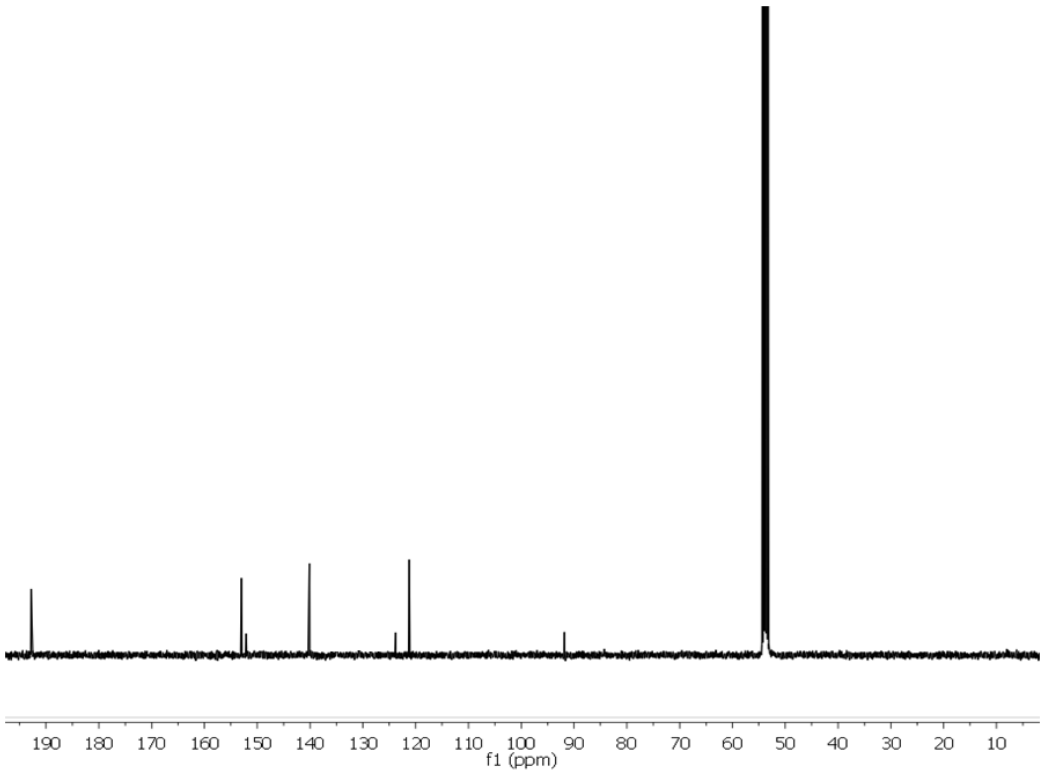

Figure S2. ^{13}C NMR of compound **4** (CD_2Cl_2, 100 MHz, 298 K).

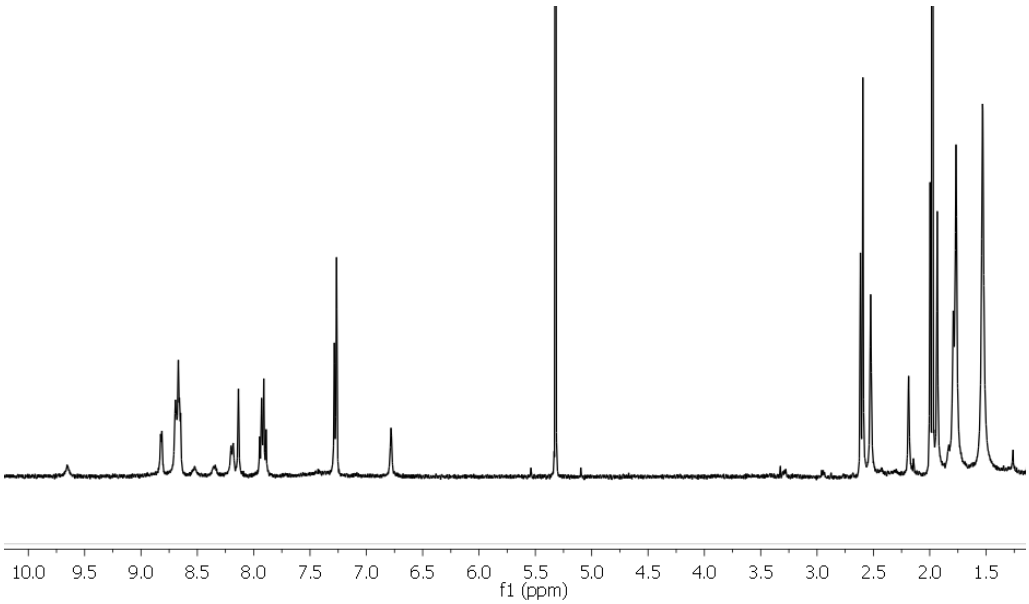

Figure S3. ^{1}H NMR of **T** (CD_2Cl_2, 400 MHz, 298 K).

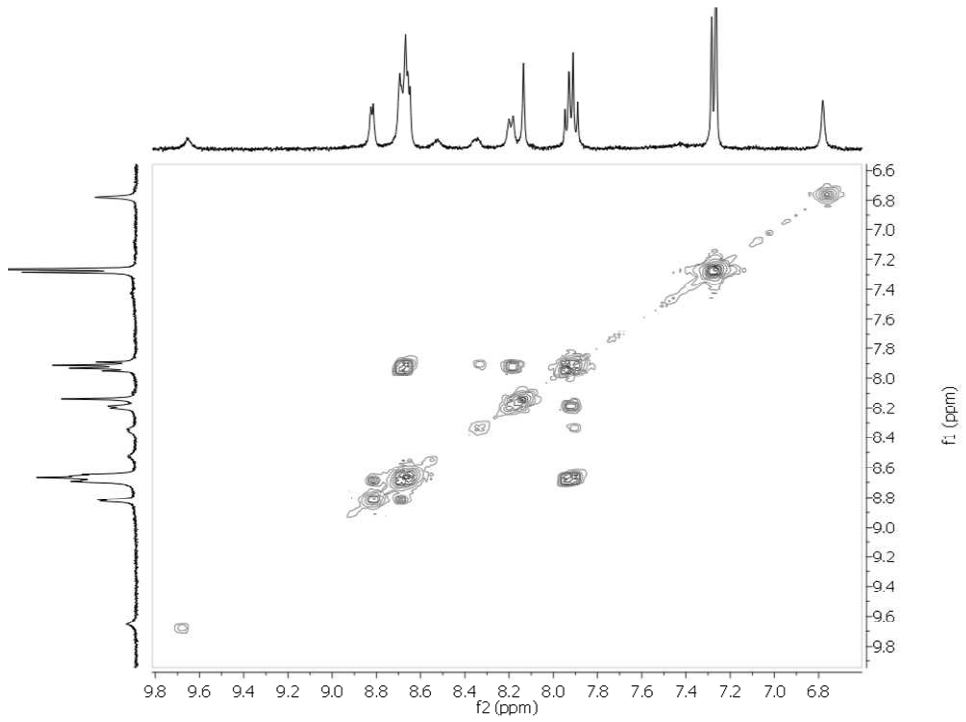

Figure S4. ^{1}H-^{1}H COSY of **T** (CD_2Cl_2, 400 MHz, 298 K).

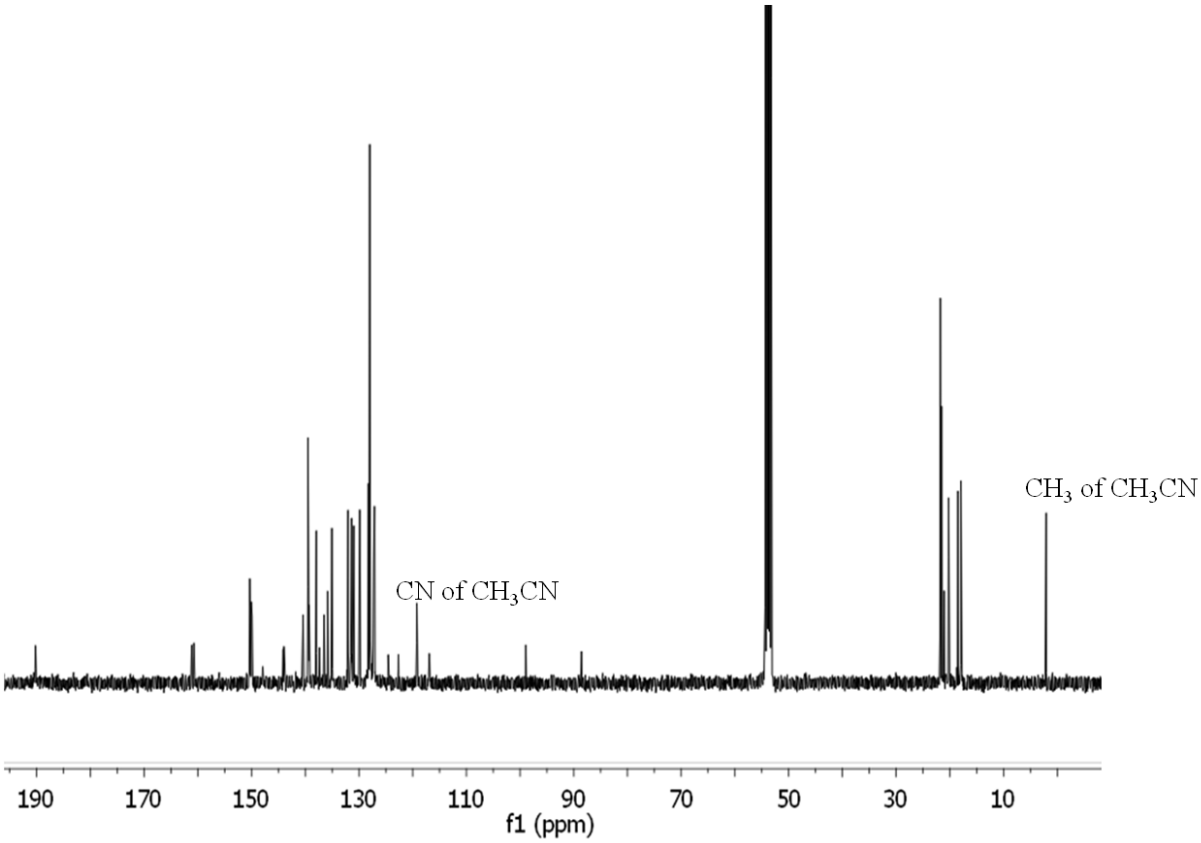

Figure S5. ^{13}C NMR of **T** (CD_2Cl_2, 100 MHz, 298 K).

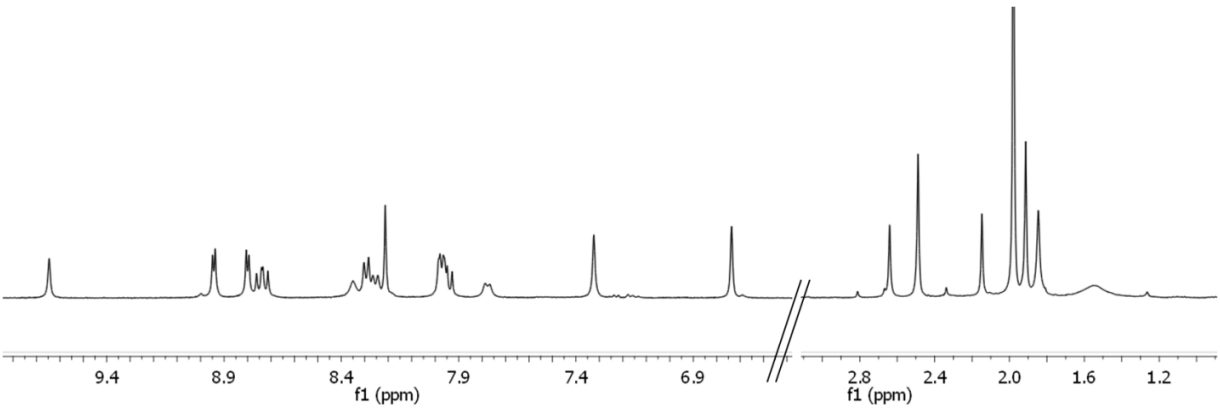

Figure S6. ^{1}H NMR of **G** (CD_2Cl_2, 400 MHz, 298 K).

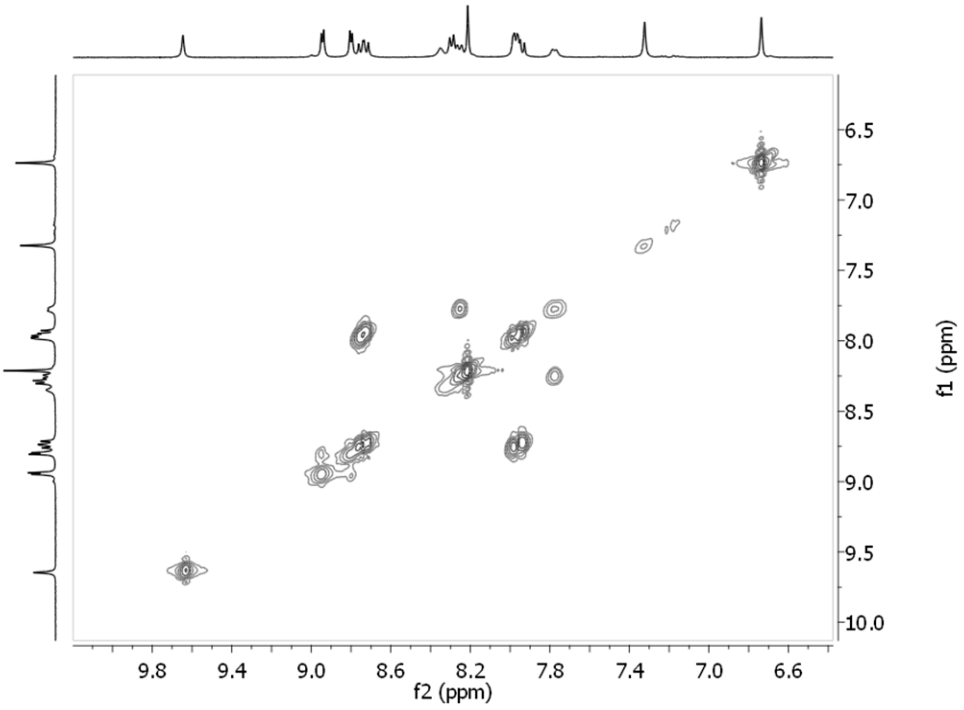

Figure S7. ^{1}H-^{1}H COSY of **G** (CD_2Cl_2, 400 MHz, 298 K).

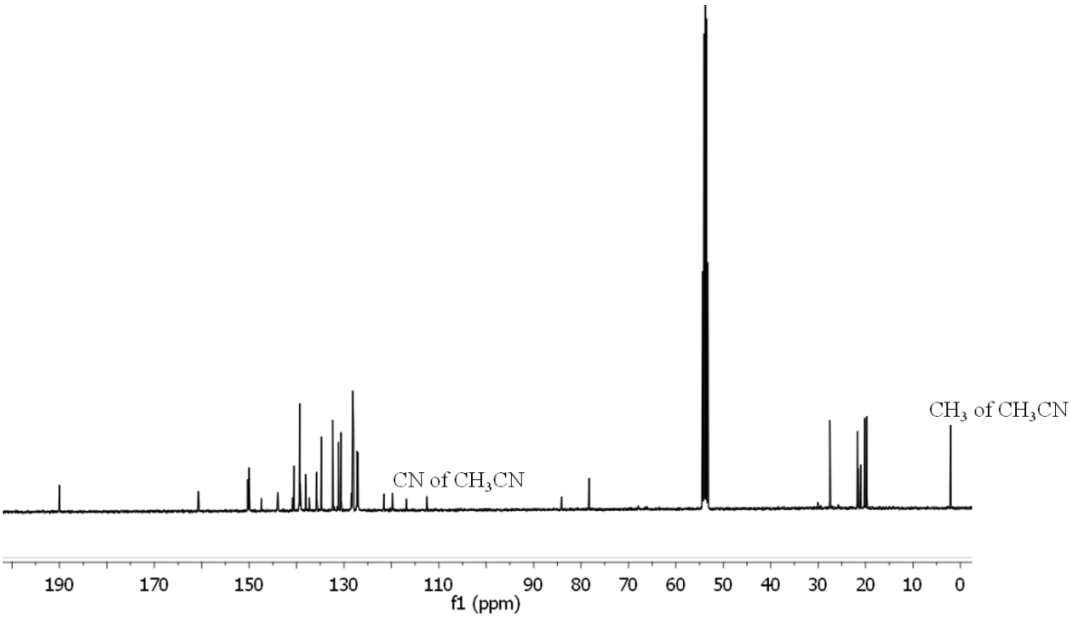

Figure S8. ^{13}C NMR of **G** (CD_2Cl_2, 100 MHz, 298 K).

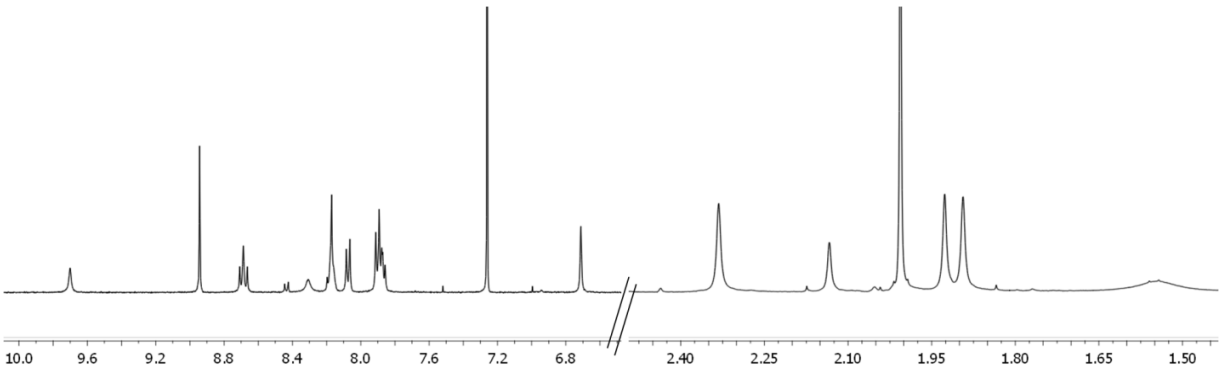

Figure S9. ^{1}H NMR of **P** ($CDCl_3$, 400 MHz, 298 K).

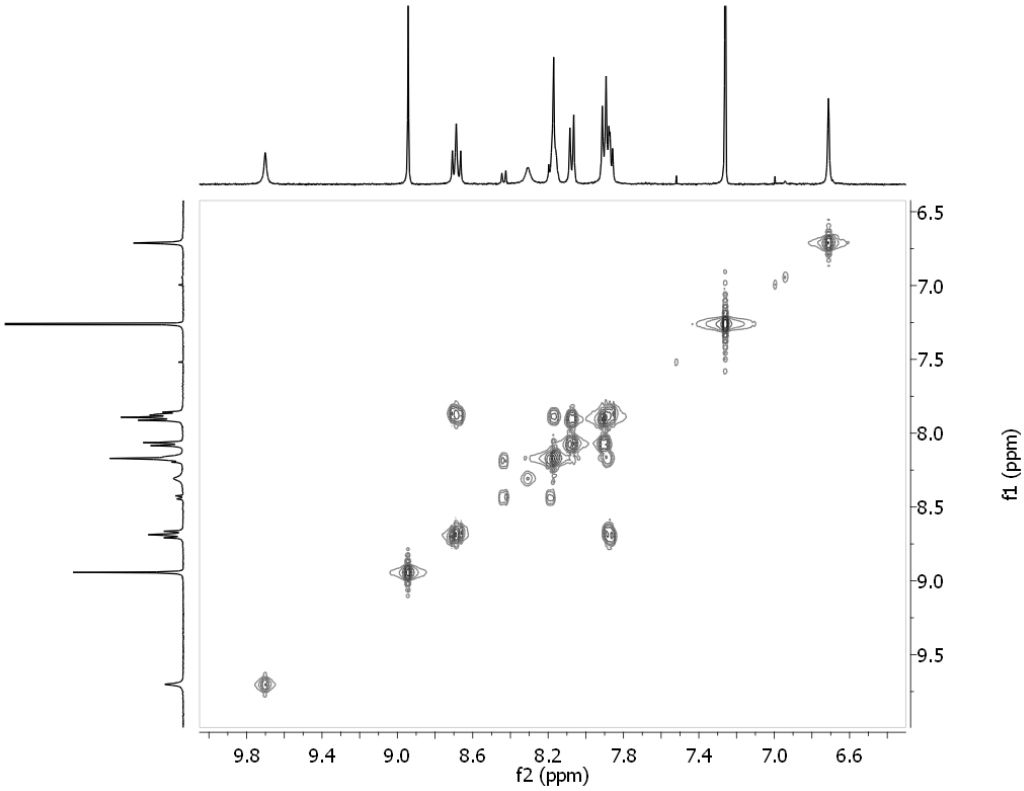

Figure S10. ^{1}H-^{1}H COSY of **P** ($CDCl_3$, 400 MHz, 298 K).

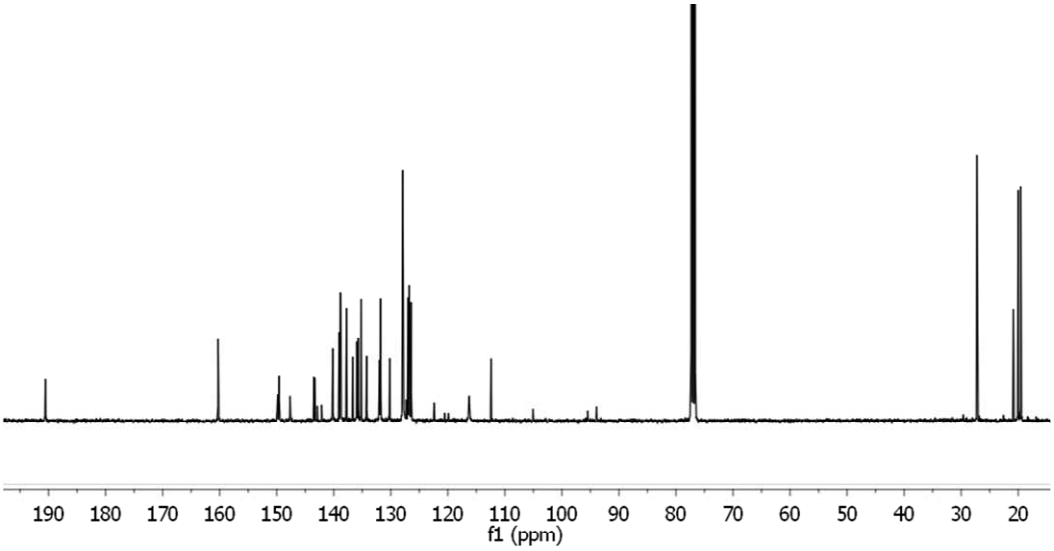

Figure S11. ^{13}C NMR of **P** ($CDCl_3$, 100 MHz, 298 K).

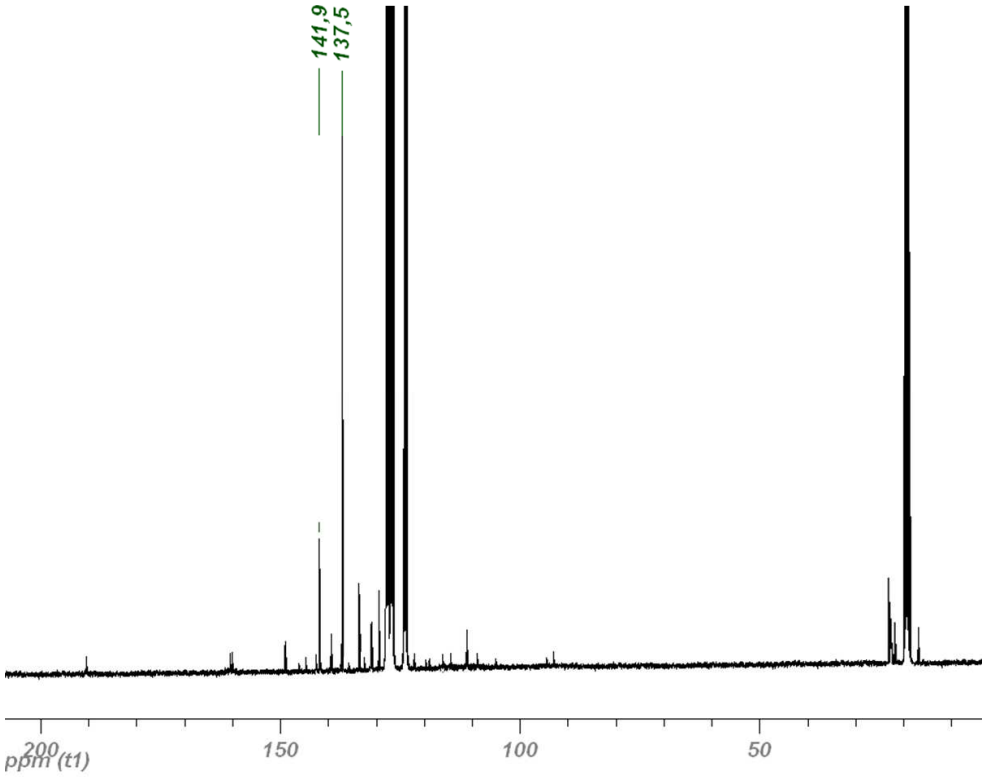

Figure S12. ^{13}C NMR of C_{60}@**T** (toluene-d_8, 100 MHz, 298 K).

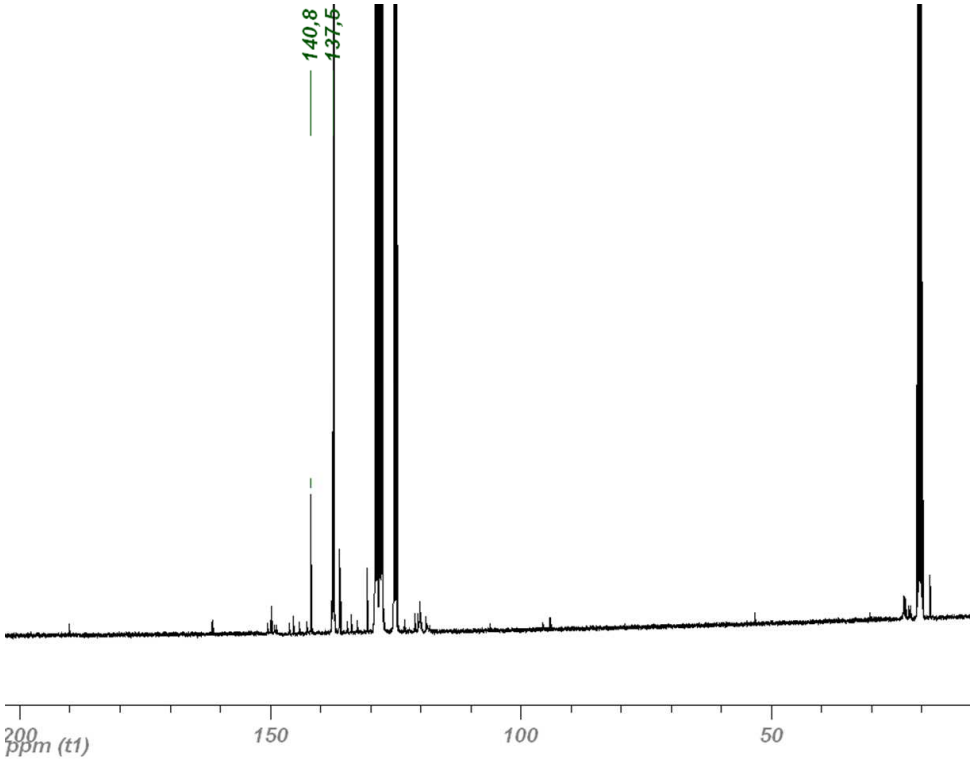

Figure S13. ^{13}C NMR of C_{60}@**G** (toluene-d_8, 100 MHz, 298 K).

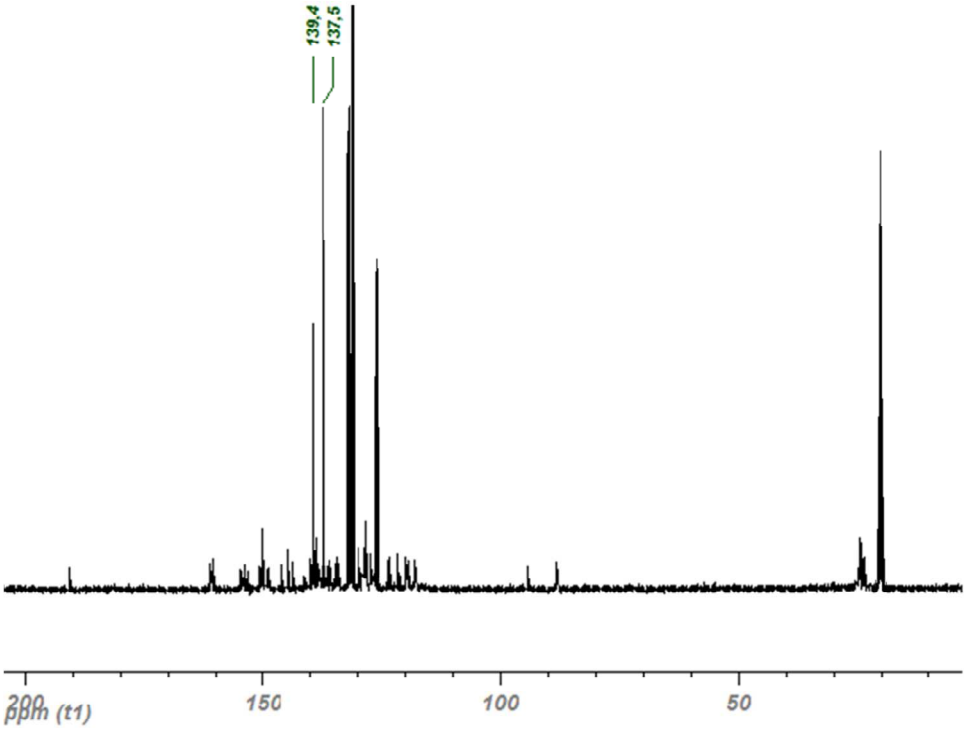

Figure S14. ^{13}C NMR of C_{60}@**P** (toluene-d_8, 100 MHz, 298 K)

ESI-MS

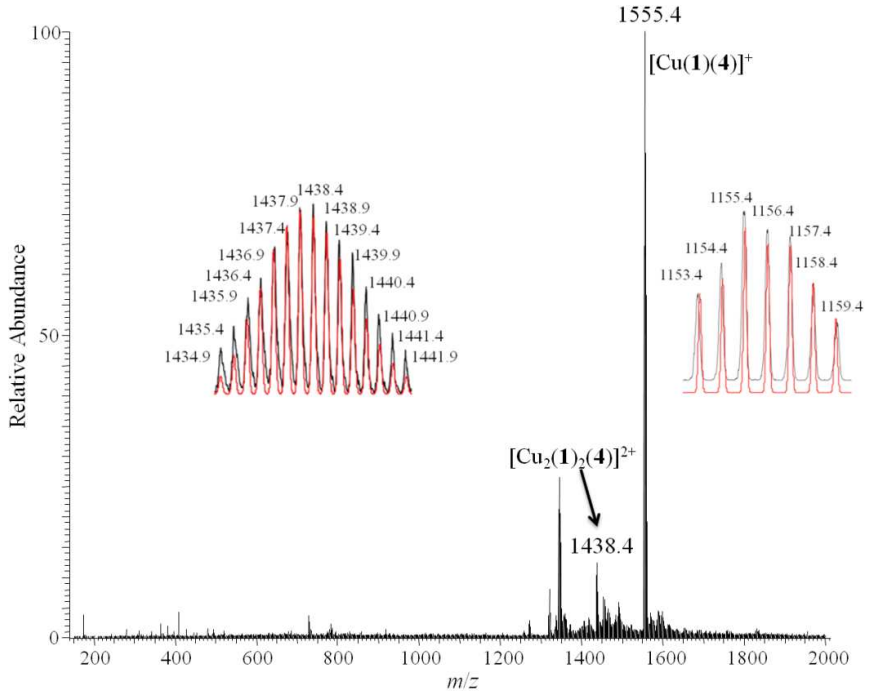

Figure S15. ESI-MS spectrum of **T**.

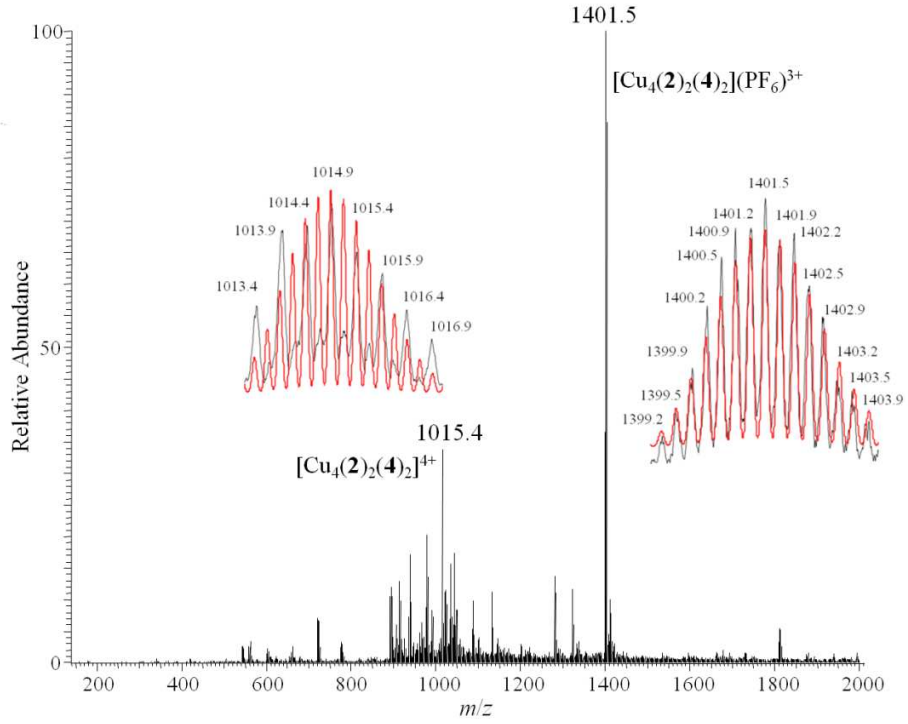

Figure S16. ESI-MS spectrum of **G**.

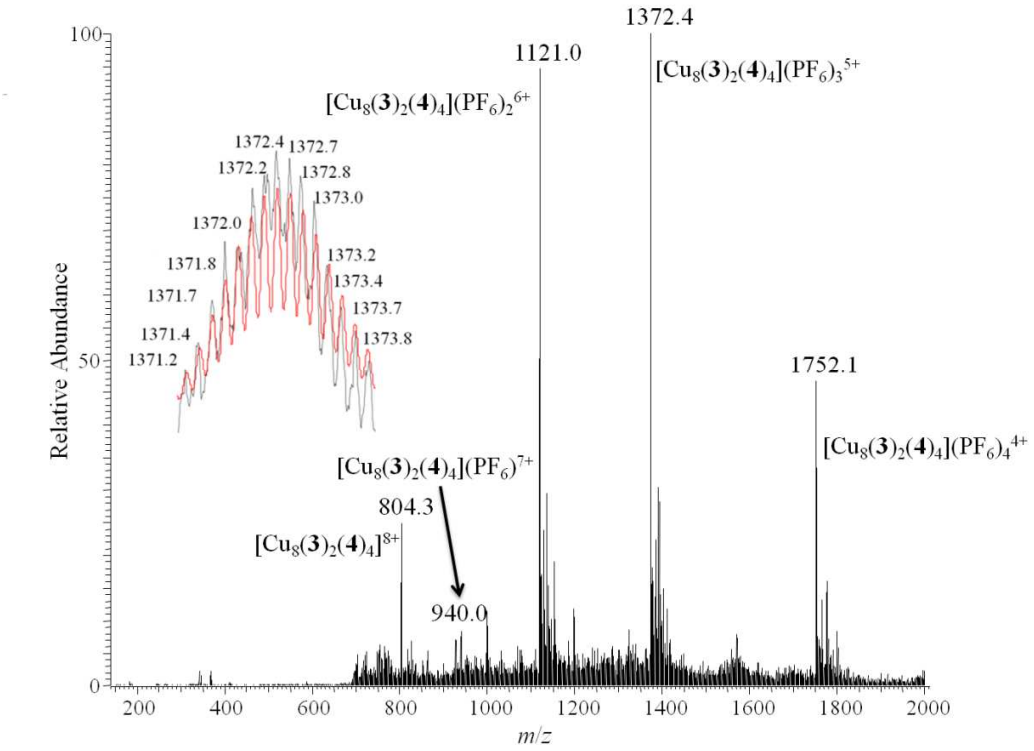

Figure S17. ESI-MS spectrum of **P**.

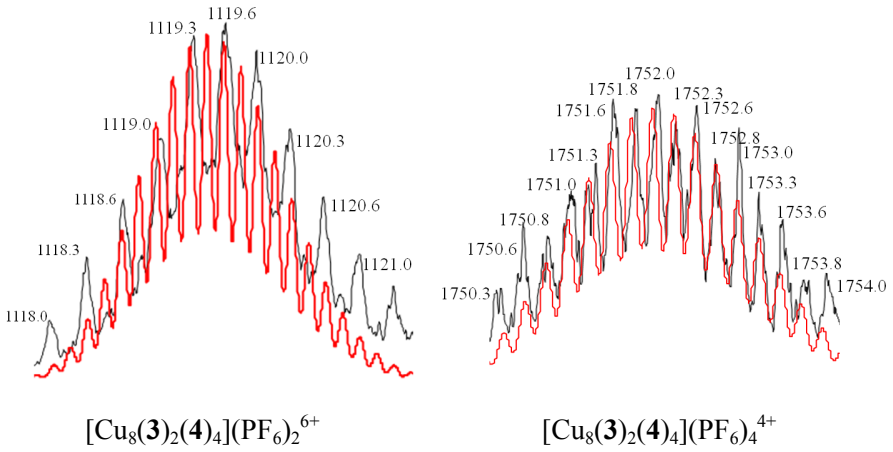

Figure S18. Experimental isotopic distributions (black lines) along with calculated isotopic distributions (red lines) for various charged species obtained after loss of the counter anions in the ESI-MS of **P**.

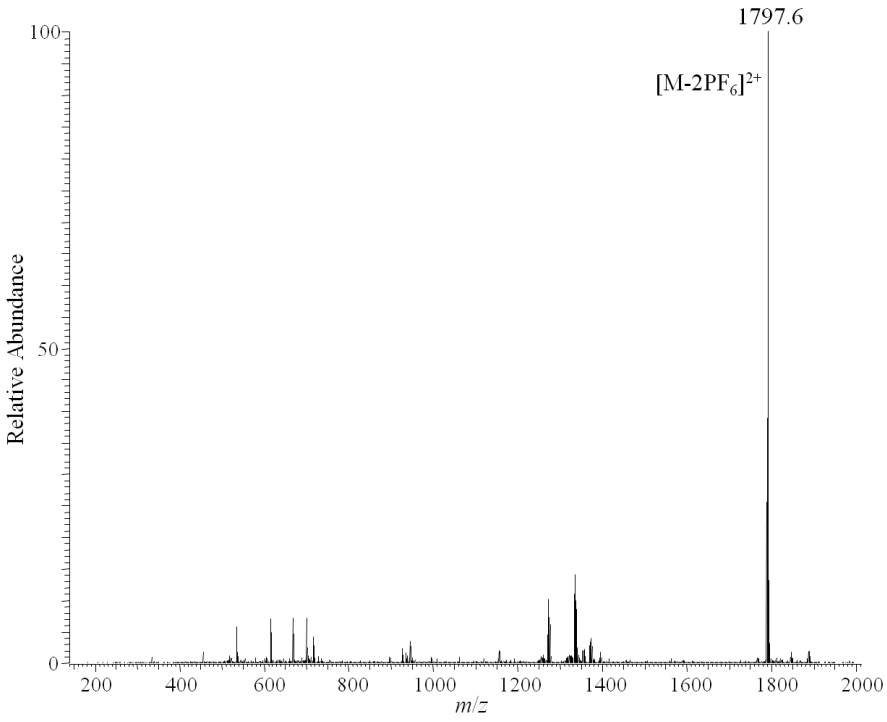

Figure S19. ESI-MS spectrum of C_{60}@**T** (= **M**) complex.

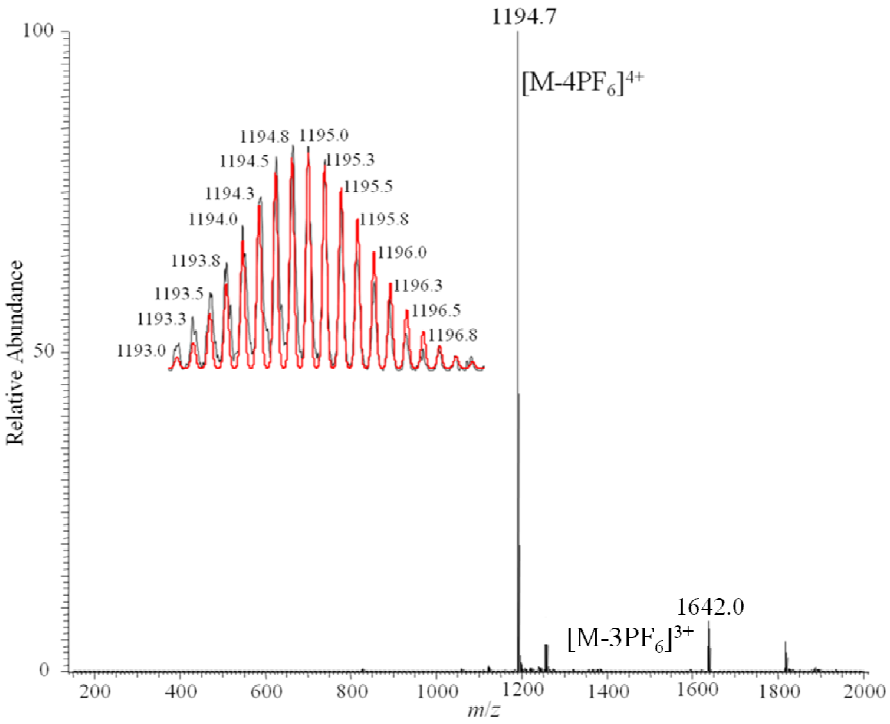

Figure S20. ESI-MS spectrum of C_{60}@**G** (= **M**) complex.

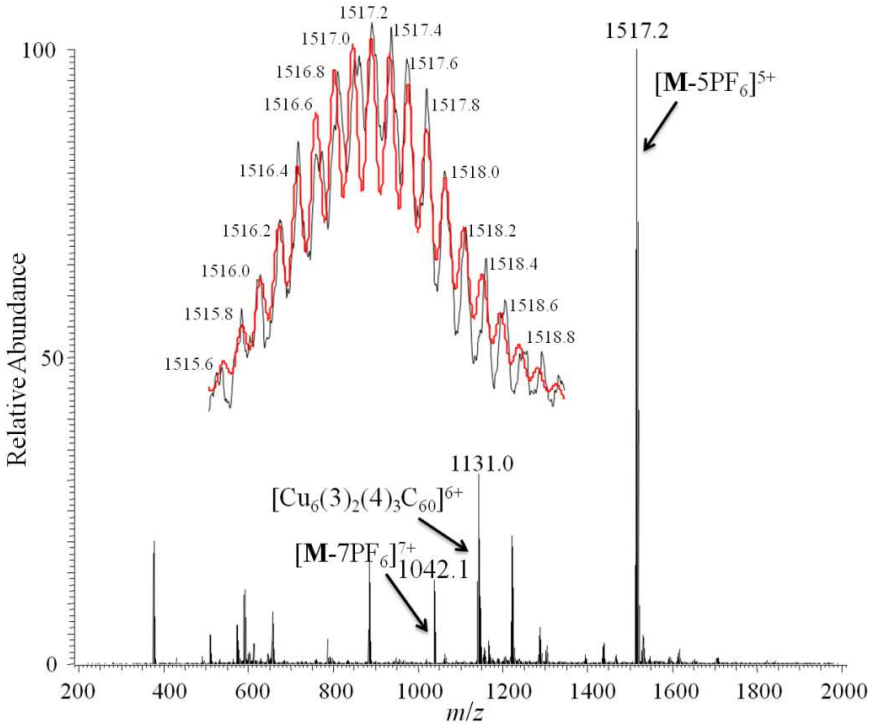

Figure S21. ESI-MS spectrum of C_{60}@**P** (= **M**) complex.

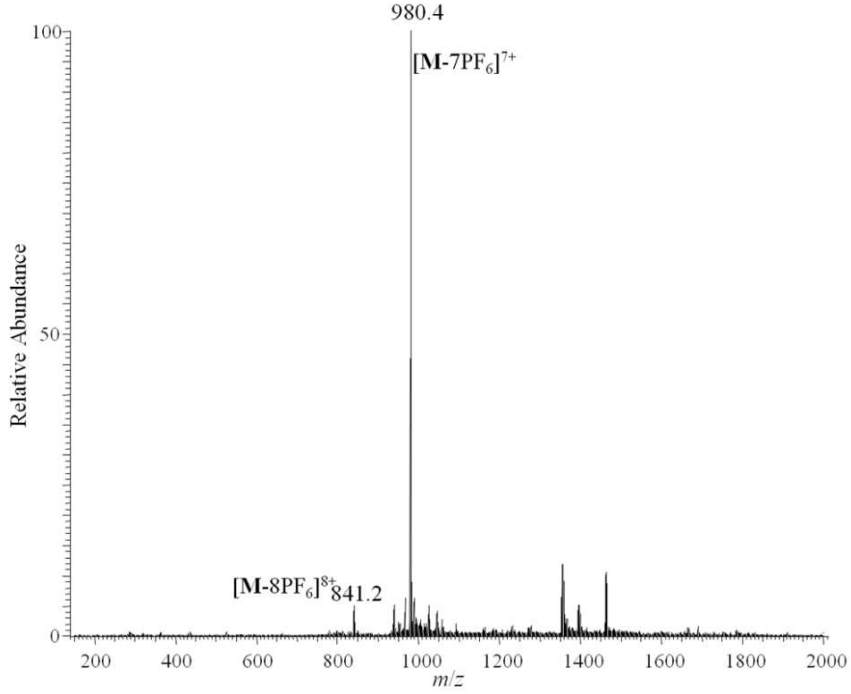

Figure S22. ESI-MS spectrum of coronene@**P** (= **M**) complex.

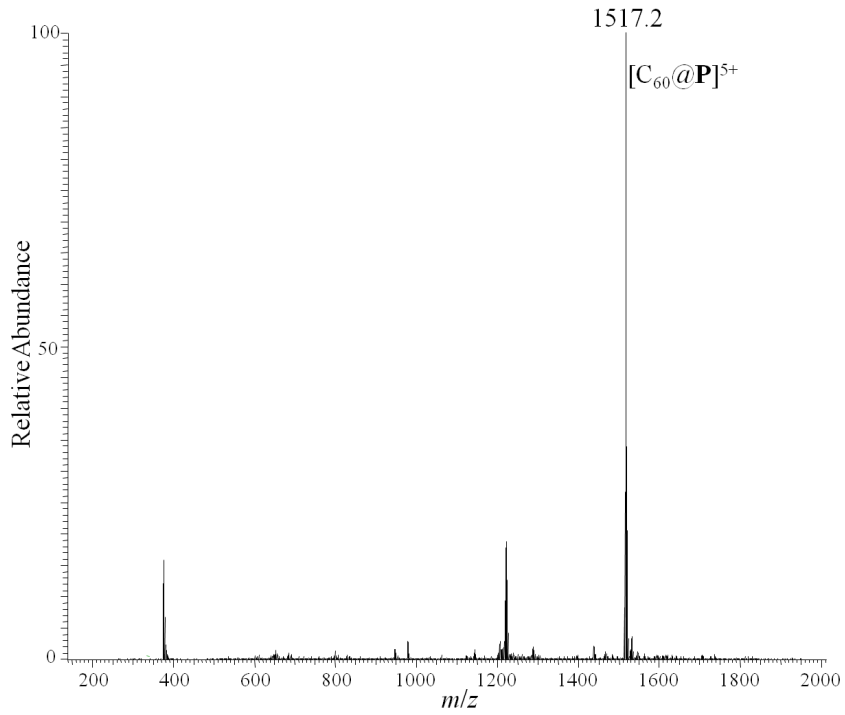

Figure S23. ESI-MS spectrum of mixture of coronene@**P** with C_{60} after refluxing for 2h.

Absorption Spectral Data

K_{assoc} values were evaluated by applying nonlinear curve-fitting to absorbance changes (ΔAbs) observed for the host upon titration with C_{60} or coronene:

$$\Delta Abs = (L(1 + K_{assoc}X + K_{assoc}A) - (L^2(K_{assoc}X + K_{assoc}A + 1)^2 - 4K_{assoc}^2AXL^2)^{0.5})/2K_{assoc}A$$

where X and A represent $[Guest]_{total}$ and $[Host]_{total}$, respectively; L denotes ΔAbs at 100% complexation; L and K_{assoc} are parameters.

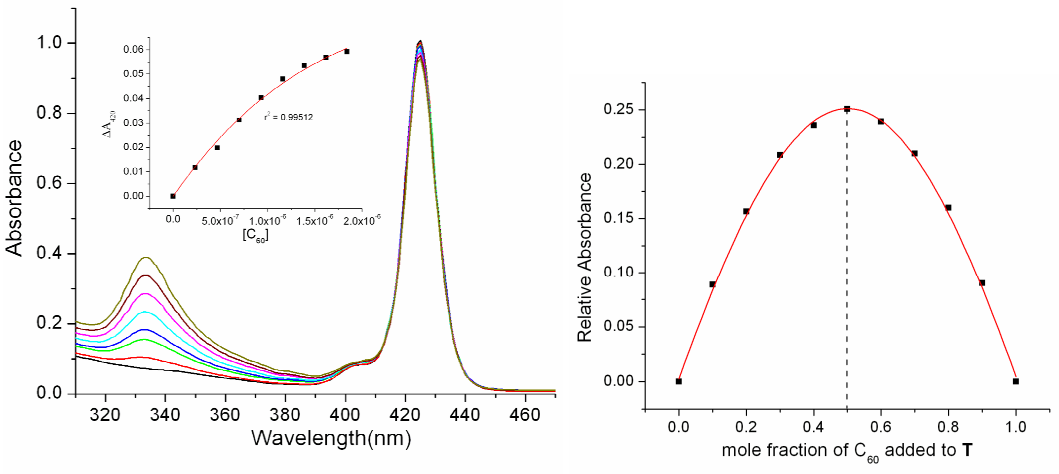

Figure S24. (Left) Absorption changes of **T** in toluene at 298 K upon titration with C_{60}. (Inset : nonlinear curve-fitting of UV-vis absorption data at λ = 420 nm: K_{assoc} = (2.9 ± 0.3) × 10^4 M^{-1}). (Right) Job plot analysis using UV-vis absorption data for C_{60}@**T** complex at λ = 420 nm.

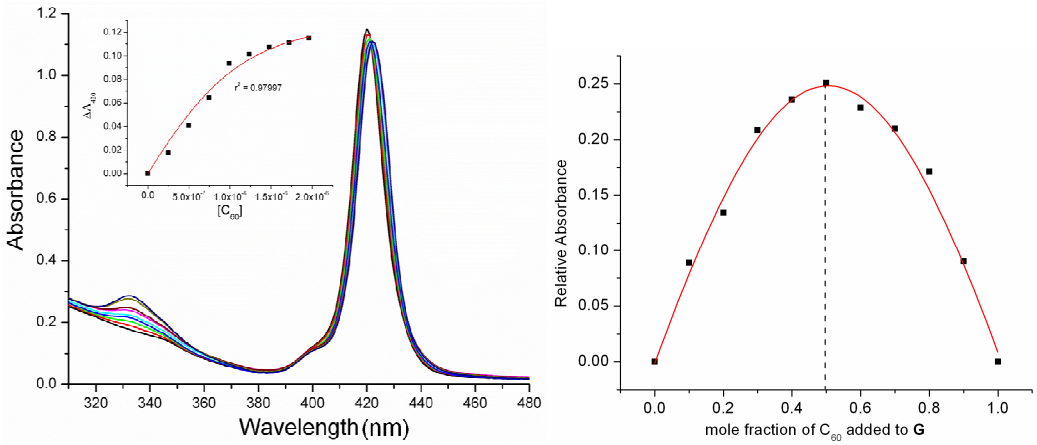

Figure S25. (Left) Absorption changes of **G** in toluene at 298 K upon titration with C_{60}. Inset: Nonlinear curve fitting of the UV-vis absorption data at λ = 420 nm: K_{assoc} = (9.1 ± 0.4) × 10^4 M^{-1}). (Right) Job plot analysis using UV-vis absorption data for C_{60}@**G** complex at λ = 420 nm.

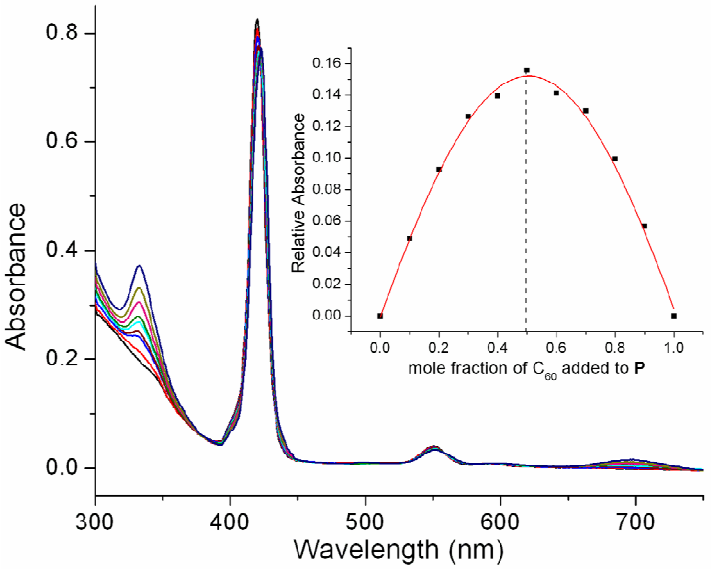

Figure S26. Absorption changes of **P** in toluene at 298 K upon titration with C_{60}: K_{assoc} = (3.3 ± 0.3) × 10^6 M^{-1}. Inset: Job plot analysis using UV-vis absorption data for C_{60}@**P** complex at λ = 420 nm.

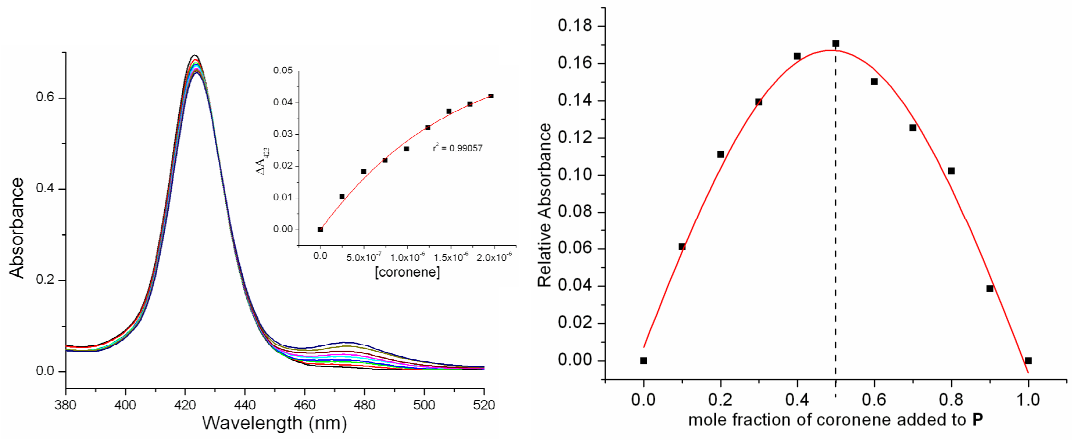

Figure S27. (Left) Absorption changes of **P** in CH_2Cl_2 at 298 K upon titration with coronene. Inset: Nonlinear curve fitting of the UV-vis absorption data at λ = 420 nm: K_{assoc} = (1.1 ± 0.6) × 10^4 M^{-1}). (Right) Job plot analysis using UV-vis absorption data for coronene@**P** complex at λ = 420 nm.

Energy Minimised Structures

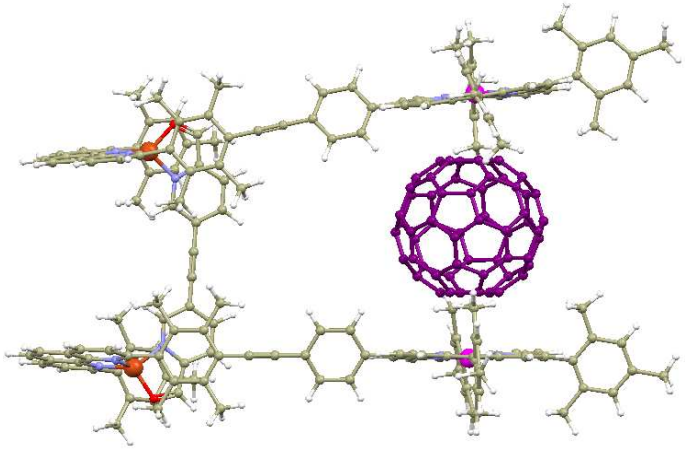

Figure S28. MM+ computed structure of C_{60}@**T**.

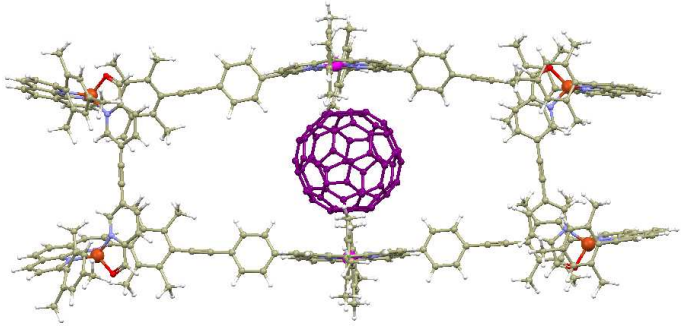

Figure S29. MM+ computed structure of C_{60}@**G**.

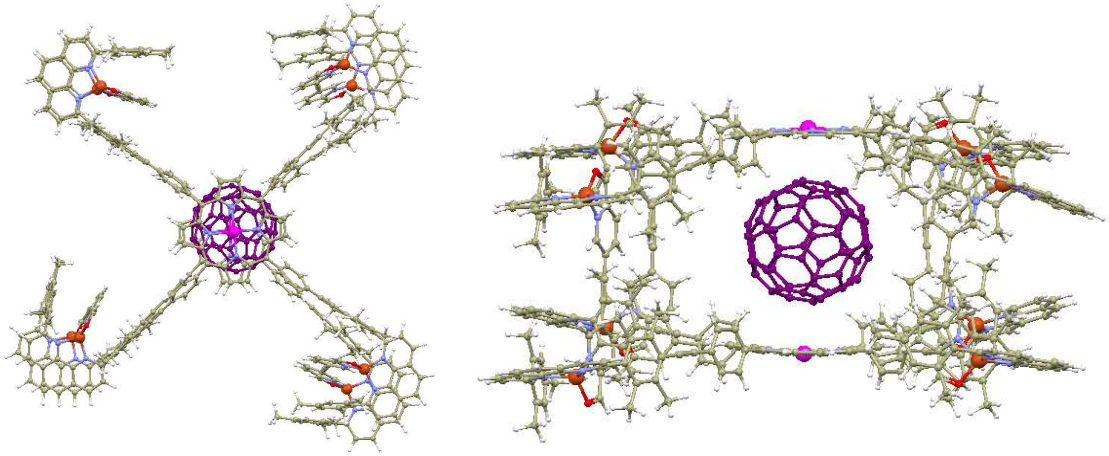

Figure S30. MM+ computed structure of C_{60}@**P**. (left) topview and (right) sideview.

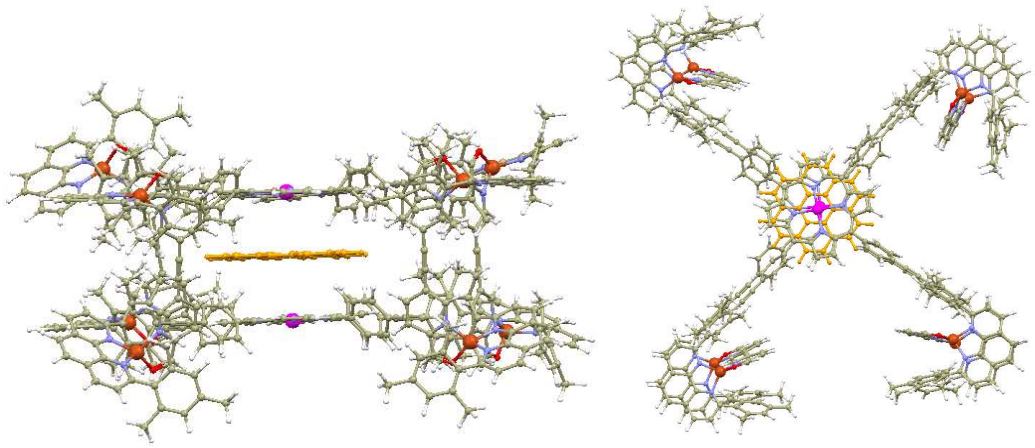

Figure S31. MM+ computed structure of coronene@**P**, (left) sideview and (right) topview.

DOSY NMR

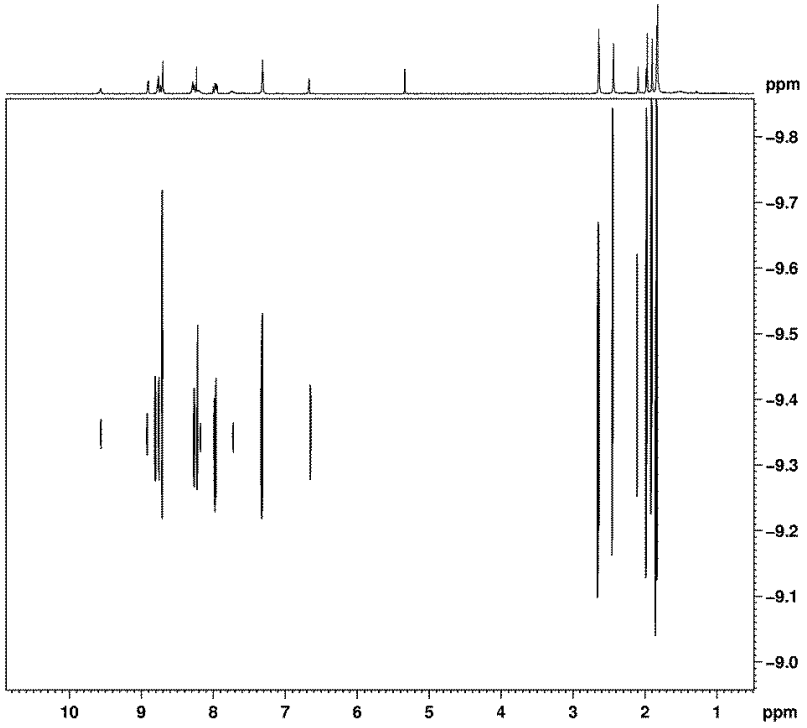

Figure S32. ^{1}H DOSY of **T** in CD_2Cl_2.

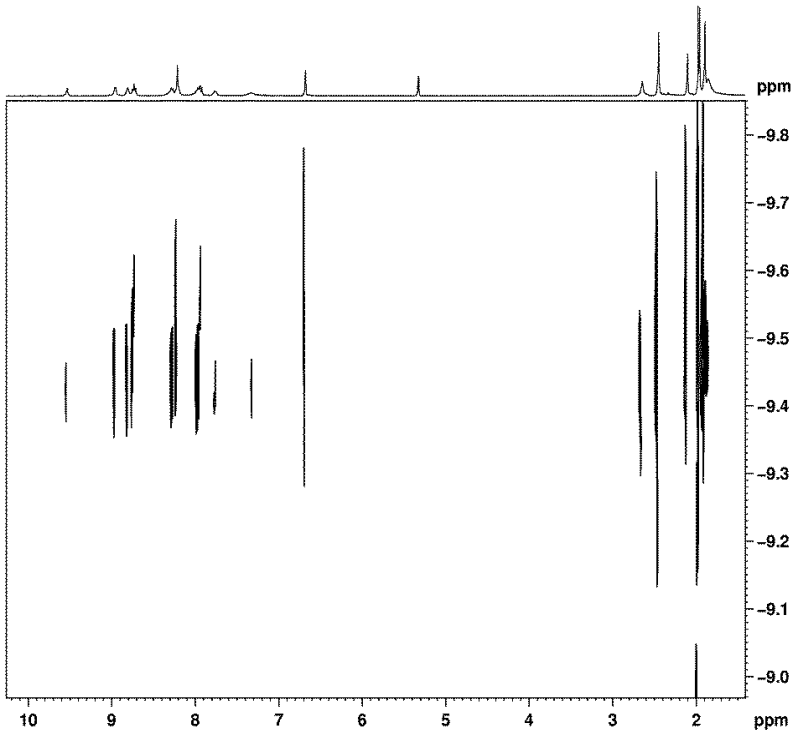

Figure S33. ^{1}H DOSY of **G** in CD_2Cl_2.

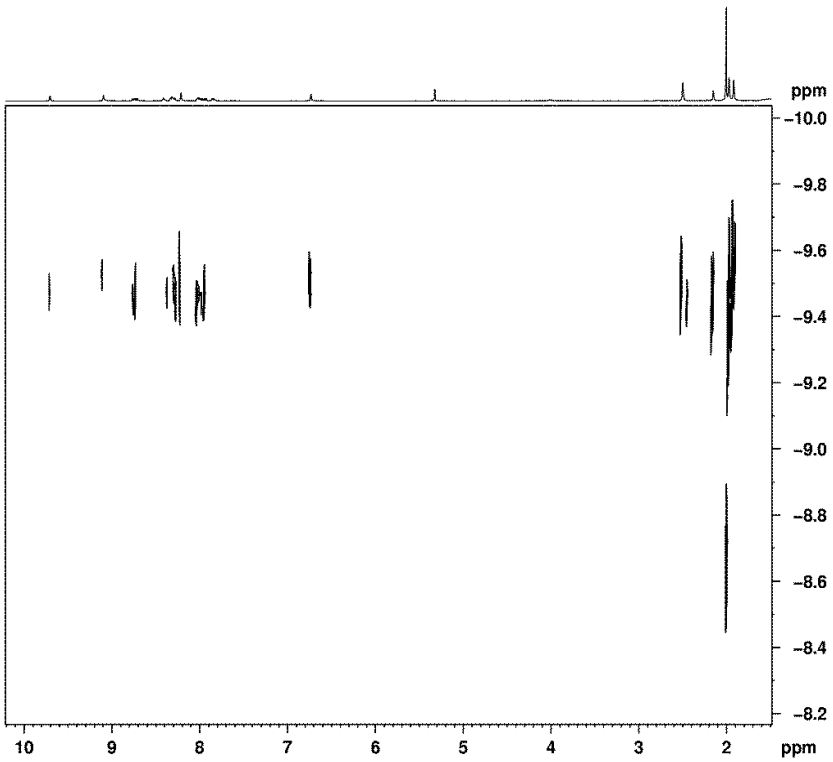

Figure S34. ^{1}H DOSY of **P** in CD_2Cl_2.